Correlation driven Mott-insulator-to-metal transition

Rubem Mondaini[1,2] and Thereza Paiva[3]
[1] *Department of Physics, Georgetown University, Washington, District of Columbia 20057, USA*
[2] *Physics Department, The Pennsylvania State University, 104 Davey Laboratory, University Park, Pennsylvania 16802, USA and*
[3] *Instituto de Física, Universidade Federal do Rio de Janeiro Cx.P. 68.528, 21941-972 Rio de Janeiro RJ, Brazil*

We study transport properties of the half-filled two-dimensional ($2D$) Hubbard model with spatially varying interactions, where a pattern of interacting and non-interacting sites is formed. We use Determinantal Quantum Monte Carlo method to calculate the double occupation, effective hopping and Drude weight. These data point to two phase transitions, driven by fermionic correlations. The first is the expected metal to a Mott insulating state. The second one, is an exotic transition from a Mott insulating state to a highly anisotropic metal, that takes place at large values of the fermion-fermion interaction. This second transition occurs when the layers formed by the spatially varying interactions decouple due to the suppression of the hopping between interacting and non-interacting sites, leading to fermionic transport along the non-interacting ones.

PACS numbers: 71.10.Fd 71.30.+h 71.27.+a

Metal insulator transitions have been a topic of intense study over many years[1]. When the transition from a metallic into an insulating state is driven by correlations it is known as the Mott transition [2, 3]. The experimental observation of the Mott insulating state in two-flavor mixtures of fermionic atoms loaded on optical lattices, [4, 5] opened new possibilities in this field. Models that take correlation effects in tight-binding systems, such as the Hubbard model, have been widely used to describe different types of insulating phases and metal-insulator transitions.

An interesting point that has been addressed in the literature is whether these same correlations could drive an insulating system metallic. When a periodic on-site energy is distributed in the system, we have the so called Ionic Hubbard Model. In the non-interacting limit, the periodic potential produces a dispersion relation that is gapped at half-filling. In these systems, correlations are responsible for a band-insulator to metal transition. [6–8].

The same on-site energies can be randomly distributed throughout the lattice, leading to an Anderson insulator [9, 10] depending on the strength of the disorder and system dimensionality. The use of speckle noise [11, 12] in cold atoms loaded on optical lattices has enabled a new experimental route to understanding the interplay between disorder and interactions. This is still an area of intense debate, with many open questions. Nonetheless, numerical data for the Anderson-Hubbard model points to an Anderson insulator to metal transition driven by correlations [13].

Can correlations drive a *Mott insulator* into a metal? Here we show that, when the interactions are not homogeneously distributed in the system, but instead are spatially varying, this correlation induced Mott insulator to metal transition can indeed take place. Although spatially varying interactions are not yet available on optical lattices, they have recently become available in ultracold gases. The ability to control a magnetic Feshbach resonance with laser light [14], has increased the tunability of interactions for bosonic systems. Submicron spatial modulation of the interaction was already achieved in a ^{174}Yb Bose-Einstein condensate [15]. Optical control of Feshbach resonances for a fermionic ultracold gas [16] has also been proposed.

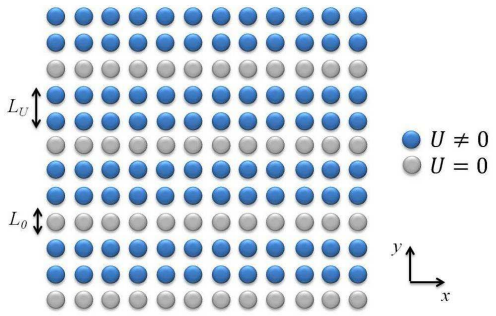

FIG. 1: (Color online) Schematic figure of the spatially varying interactions in a system with $L_U = 2$ $L_0 = 1$ in a 12×12 lattice.

Here we consider a modified version of the Hubbard Model (HM) with spatially varying interactions, whose Hamiltonian reads

$$\mathcal{H} = -t \sum_{\langle i,j\rangle,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + \sum_i U_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right) - \mu \sum_{i,\sigma} n_{i\sigma}, \quad (1)$$

where, in standard notation $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) creates (destroys) a fermion in site i in state σ. The hopping parameter between nearest neighbor sites ($\langle i,j\rangle$) is set to $t = 1$, U_i is the site dependent interaction, and μ is the chemical potential controlling the band filling to yield a given fermionic density ρ. The interaction term is written in particle-hole symmetric form. Thus, tuning $\mu = 0$ drives the occupation to one in every site for all Hamiltonian

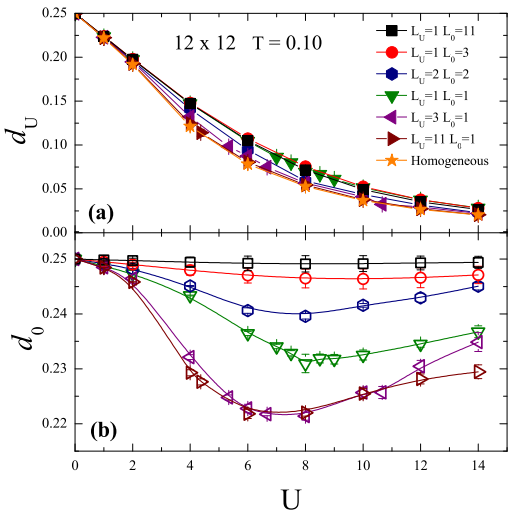

FIG. 2: (Color online) Double occupation within (a) repulsive (d_U) and (b) non-interacting sites (d_0) as a function of U for different 12×12 superlattices at $T = 0.10$. Double occupation for the corresponding homogeneous system (stars) is also shown in (a) for comparison.

parameters t, U_i and temperatures T. We have here restricted our study to half-filled systems. To simulate the spatially modulated systems we construct a layered pattern of repulsive and non-interacting layers where $U > 0$ and $U = 0$, respectively. We define the width of the repulsive layer as L_U and that of the non-interacting one as L_0 as depicted in Fig. 1 for a $L_U = 2$ $L_0 = 1$ in a 12×12 lattice. Note that not all patterns fit all the available lattice sizes. Here we use Determinantal Quantum Monte Carlo (DQMC) simulations [19] to probe transport properties of the half-filled two-dimensional square $L \times L$ system with spatially varying interactions. Metal-insulator transitions of one-dimensional non-symmetrical Hubbard superlattices [17] were studied and shown to have an interesting behavior where the Mott transition takes place away from half-filling, at a pattern dependent density [18].

A quantity of interest is the double occupation $d = \langle n_\uparrow n_\downarrow \rangle$, as it is measured in optical lattices experiments. Indeed, it has been used to probe metal insulator transitions [5] in fermionic two-flavor mixtures of ^{40}K atoms. For the homogeneous, non-interacting, metallic system $d = \langle n_\uparrow \rangle \langle n_\downarrow \rangle = 0.25$. As correlations are turned on at a fixed temperature, d decreases, signaling the metal-insulator transition, and approaches 0 as $U \to \infty$. The symmetric form of the Hamiltonian requires that, at half-filling, the charge distribution is homogeneous throughout the lattice. The double occupation, on the other hand, is not homogeneous and follows the superlattice pattern. Single-atom resolved double occupation [20] is experimentally available, therefore it is then relevant to define d_0 and d_U, the average double occupation within non-interacting and interacting sites, respectively.

The U-dependence of both d_0 and d_U for different superlattice patterns and fixed temperature ($T = 0.10$) is shown in Fig. 2. Within the repulsive sites (Fig. 2(a)) d_U decreases monotonically with U, and approaches that of the corresponding homogeneous system as the ratio L_U/L_0 is increased. The behavior of d_U is in agreement with a metal-insulator transition as the interactions are turned on. The double occupation on the non-interacting sites (Fig. 2(b)) is affected by the strength of the interaction on the neighboring repulsive ones and displays a surprising non-monotonic behavior with U. Starting from $U = 0$, as U increases the effect of the interactions "leaks" into the non-interacting sites. When the ratio L_U/L_0 increases, the double occupation is reduced even where the interaction is turned off. It is worth noting the difference in the cases $L_U = 1$ $L_0 = 1$ and $L_U = 2$ $L_0 = 2$, where the ratio L_U/L_0 is the same, but the wider free layer in the latter makes the spins more uncorrelated in the non-interacting region. As $U \to \infty$ double occupations are forbidden in the repulsive sites and hopping between free and repulsive sites is completelly suppressed, leading to a decoupling between free and repulsive layers and bringing d_0 back to the value of the homogeneous non-interacting system, $d_0 \to 0.25$. The upturn in d_0 signals the onset of the decoupling between the layers, that, as we shall see bellow, leads to an insulator-to-metal transition.

We now analyze the effective hopping [21, 22], which is defined as the ratio of the kinetic energy on a superlattice to its non-interacting homogeneous counterpart value, both in the direction along (x) and across (y) the layers;

$$\frac{t_{\alpha,eff}}{t_\alpha} = \frac{\langle c^\dagger_{j+\hat{\alpha}\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{j+\hat{\alpha}\sigma} \rangle_{SL}}{\langle c^\dagger_{j+\hat{\alpha}\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{j+\hat{\alpha}\sigma} \rangle_{U=0}}, \qquad (2)$$

where $\alpha = x$ or y. One would expect that anisotropy favors the fermionic transport along the direction of the layers. This is indeed the case, as can be readily observed in Fig. 3, where the repulsive interaction splits the x and y contributions to the effective hopping, reducing $t_{y,eff}/t_y$ more strongly than $t_{x,eff}/t_x$ as U is increased. In the direction perpendicular to the layers the effective hopping approaches that of the corresponding homogeneous system, as L_U/L_0 increases, displaying the characteristic behavior of an insulating system. Along the direction of the layers, on the other hand, the effective hopping is close to that of the non-interacting metallic system when $L_U/L_0 < 1$.

We can gain further insight by analyzing the effective hopping separately within free and repulsive layers. This is done in Fig. 4, where $t^U_{x,eff}/t_x$(filled symbols) and $t^0_{x,eff}/t_x$ (empty symbols) are normalized by the number of repulsive and free sites, respectively. The effective hopping along the repulsive sites is independent of the superlattice pattern for small U and follows closely the analyt-

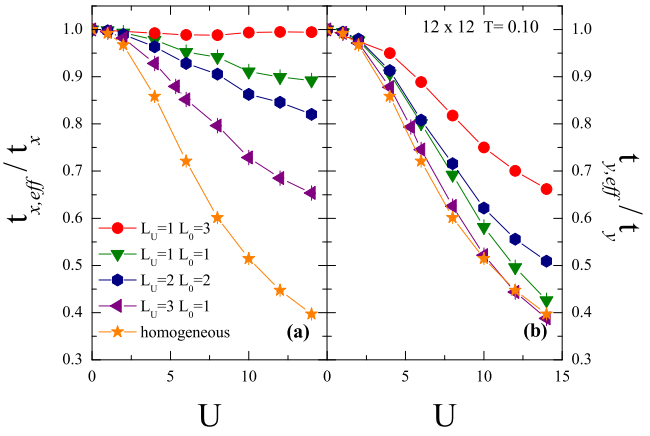

FIG. 3: (Color online) Effective hopping along (a) and across (b) the direction of the layers as a function of interaction strength U, for 12×12 superlattices at $T = 0.10$. Results for the corresponding homogeneous system (stars) are shown in both panels for comparison.

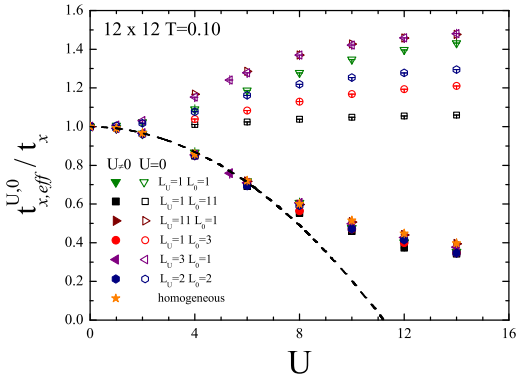

FIG. 4: (Color online) Effective hopping along free (open symbols) and repulsive (closed symbols) for 12×12 superlattices at $T = 0.10$ as a function of U. Dashed line is perturbation theory analytical result, from Ref. 21.

ical results for perturbation theory in the homogeneous system [21]. As U is increased there are small deviations from the homogeneous counterpart. From the similarity of the effective hopping in the homogeneous system and along the repulsive layers, we can infer that transport properties are essentially the same in both, leading to an insulating behavior of the fermions along the correlated layer. Therefore, the main contribution to the transport in the direction parallel to the layers comes from the non-interacting sites, where $t^0_{x,eff}/t_x > 1$. Fig. 4 shows that as U is increased the contribution to the kinetic energy due to hopping between free sites is enhanced. When comparing different patterns we can see that the enhancement in $t^0_{x,eff}$ is optimized in lattices with narrow non-interacting layers ($L_0 = 1$) separated by wide repulsive ones. The picture emerging from Fig. 4 is that, while the repulsive layers are insulating, transport along the non-interacting layers is actually improved by the presence of the neighboring repulsive sites and increasing interaction strength among them.

The effective hopping cannot be used as an order parameter for the metal-insulator transition as it only approaches zero for $U \to \infty$ in the homogeneous case, whereas the system is known to be in a Mott insulating state for any non-zero value of U. Among the available quantities to characterize the transport properties of the HM within DQMC simulations, the Drude weight is the one less affected by finite size effects [23]. It can be determined by [24]

$$\frac{D_\alpha}{\pi e^2} \equiv \lim_{T,m\to 0}[\langle -k_\alpha \rangle - \Lambda_{\alpha\alpha}(\mathbf{q} = 0, i\omega_m)], \qquad (3)$$

where $\langle k_\alpha \rangle$ is the contribution to the average kinetic energy from fermions hopping along the α direction and $\Lambda_{\alpha\alpha}(\mathbf{q} = 0, i\omega_m)$ is the long wavelength limit of the current-current correlation function with $\omega_m = 2m\pi T$ the Matsubara frequency and $\alpha = x$ or y. In principle the Drude weight as defined by (3) only provides information about the ground state of the system. Here we calculate temperature dependent approximants to D and analyze how they converge as the temperature is lowered.

The Drude weight takes different values along the two preferential directions. Across the layers it displays an insulating character for all superlattices considered (not shown) in agreement with the effective hopping behavior. In Fig. 5(a) we plot the Drude weight along the direction of the layers for a fixed system size (8×8) for different patterns as wells as for the homogeneous system. The Drude weight for the $U \neq 0$ homogeneous system (stars) shows the expected insulating behavior; as the temperature is reduced $D/\pi e^2 \to 0$ at a given temperature, we shall call T^*. For $U = 4$ (dot centered stars), $T \sim 0.2$ and for $U = 10$ (closed stars), $T^* \sim 0.85$. T^* is related to the charge gap and increases as U increases. Our values of T^* are in agreement with the results of Ref. 25 where this temperature is obtained in a completely different fashion, by the gap emergence in the spectral weight function. The negative values of D are a feature of the finite system size[24], and converge to zero in the thermodynamic limit [23]. For the non-interacting homogeneous system (open squares) $D/\pi e^2 = 0.79$ as $T \to 0$, indicating an isotropic metallic behavior.

Let us now turn to the superlattices, with an intermediate interaction strength $U = 4$ (dot centered symbols), the Drude weight goes to zero, signaling an insulating ground state; T^* depends on the interaction pattern and increases as L_U/L_0 increases, being smaller than its homogeneous counterpart. Contrary to what happens in the homogeneous system, increasing U does not increase the charge gap, see closed symbols in Fig. 5(a). For the system with $L_U = 3$ and $L_0 = 1$, T^* is roughly the same for $U = 4$ and $U = 10$, whereas for the systems with $L_U/L_0 \leq 1$ the Drude weight stabilizes at non-zero values for the lower temperatures achieved, and approaches that of the non-interacting case as L_U/L_0 is reduced.

In Fig. 5(b) we study size and temperature effects on the Drude weight for the $L_U = 1$ $L_0 = 3$ system.

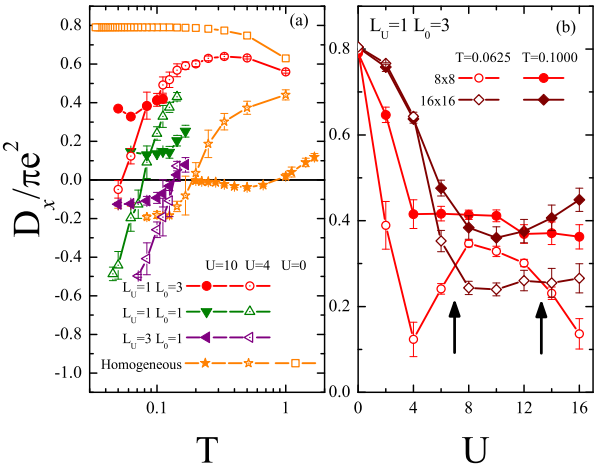

FIG. 5: (Color online) (a) Temperature dependence of the Drude weight along the direction of the layers, for 8×8 lattices for different SL's with $U = 4$ and $U = 10$ and homogeneous system with $U = 0$, 4 and 10; (b) U dependence of the Drde weight for the $L_U = 1$ $L_0 = 1$ superlattice at $T = 0.0625$ and $T = 0.1000$.

As $D_x/\pi e^2$ evolves with U we can divide the system's behavior in three regions, determined by the crossings between 8×8 and 16×16 data. Let us call the values of U where the crossings take place U_{C1} and U_{C2}. For $U < U_{C1}$ one can see that $D_x/\pi e^2$ is larger for the larger system size, pointing to a non-zero contribution as $T \to 0$ and $L \to \infty$, the characteristic metallic behavior. For $U_{C1} < U < U_{C2}$ we have the opposite behavior; as the system size is increased, the Drude weight decreases, leading to a vanishing contribution in the thermodynamic limit. Note that this insulating region increases as the temperature decreases. As U increases even further and the region beyond U_{C2} is reached, the behavior is similar to that of the first region: $D_x/\pi e^2$ is larger for the larger system size, and the system is once again metallic. The values of U_{C1} and U_{C2} depend on temperature and are a likely to change when larger system sizes are considered. Nonetheless, the existence of two critical U values leading to a metal to Mott insulator transition for small U, followed by a transition from an insulating to a metallic state along the direction of the layers at large U is supported not only by the Drude weight data, but also from the effective hopping and double occupation.

In summary, we have employed Determinantal Quantum Monte Carlo simulations to study the effect of spatially varying interactions in two dimensional half-filled systems strongly interacting fermions. We have found that, as expected, when interactions are turned on the system undergoes a metal to Mott insulator transition. Although the system is particle-hole symmetric and charge is evenly distributed among free and repulsive sites, the double occupation is not constant throughout the lattice. Double occupation on non-interacting sites are influenced by the neighboring repulsive sites, first decreasing as U increases and then increasing to return to the uncorrelated value as $U \to \infty$. This upturn in the double occupation signals the decoupling between free and repulsive layers that takes place at large values of U. Evidence from double occupation, effective hopping and Drude weight show that, when this decoupling occurs, the system undergoes an exotic transition from a Mott insulator to metal, driven by fermionic correlations. We hope this results will encourage the experimental realization of such spatially varying interactions in optical lattices.

We are grateful to R. R. dos Santos and R. T. Scalettar for useful discussions. Financial support from the Brazilian agencies CNPq, CAPES, FAPERJ, and INCT on Quantum Information is gratefully acknowledged.

[1] Conductor Insulator Quantum Phase transitions, edited by V. Dobrosavljevic, N. Trivedi and J. M. Valles, Jr; Oxford University Press, Oxford (2012).
[2] N. F. Mott, Proc. Phys. Soc. **A 62**, 416 (1949); Metal-Insulator Transitions, 2nd ed. Taylor and Francis, London, (1990).
[3] M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. **70**, 1039 (1998).
[4] U. Schneider, L. Hackermuller, S. Will, Th. Best, I. Bloch, T. A. Costi, R. W. Helmes, D. Rasch, A. Rosch, Science **322**, 1520 (2008).
[5] R. Jördens, N. Strohmaier, K. Günter, H. Moritz, and T. Esslinger, Nature **455**, 204 (2008).
[6] N. Paris, K. Bouadim, F. Hebert, G. G. Batrouni, and R. T. Scalettar, Phys. Rev. Lett. **98**, 046403 (2007).
[7] A. Garg, H. K. Krishnamurthy, and M. Randeria, Phys. Rev. Lett. **97**, 046403 (2006).
[8] S. S. Kancharla, and E. Dagotto, Phys. Rev. Lett. **98**, 016402 (2007).
[9] P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).
[10] D. Belitz and T. R. Kirkpatrick, Rev. Mod. Phys. **66**, 261 (1994).
[11] J. Billy, V. Josse, Z. Zuo, A Bernard, B. Hambrecht, P Lugan, D. Clément, L. Sanchez-Palencia, P. Bouyer, and A. Aspect, Nature **453**, 891 (2008).
[12] M. White, M. Pasienski, D. McKay, S. Q. Zhou, D. Ceperley, and B. DeMarco, Phys. Rev. Lett. **102**, 055301 (2009).
[13] M. Ulmke, V. Janis, D. Vollhardt, Phys. Rev. B **51**, 10411 (1995).
[14] D. M. Bauer, M. Lettner, C. Vo, G. Rempe, and S. Dürr Nature Phys. **5**, 339 (2009).
[15] R. Yamazaki, S. Taie, S. Sugawa, and Y. Takahashi, Phys. Rev. Lett. **105**, 050405 (2010).
[16] H. Wu and J. E. Thomas, Phys. Rev. Lett. **108**, 010401 (2012); H. Wu and J. E. Thomas, Phys. Rev. A **86**, 063625 (2012).
[17] T. Paiva, R. R. dos Santos Phys. Rev. Lett. **58**, 1126 (1996).
[18] T. Paiva, R. R. dos Santos Phys. Rev. B **76**, 9607 (1998).
[19] R. Blankenbecler, R. L. Sugar and D. J. Scalapino, Phys. Rev. D **24**, 2278 (1981).
[20] J. F. Sherson, C. Weitenberg, M. Endres, M. Cheneau, I. Bloch, and S. Kuhr, Nature **467**, 68 (2010).

[21] S. R. White, D. J. Scalapino, R. L. Sugar, E. Y. Loh, J. E. Gubernatis, and R. T. Scalettar, Phys. Rev. B **40**, 506 (1989).
[22] C. N. Varney, C.R. Lee, Z. J. Bai, S. Chiesa, M. Jarrell, and R. T. Scalettar, Phys. Rev. B **80**, 075116 (2009).
[23] R. Mondaini, K. Bouadim, T. Paiva and R. R. dos Santos, Phys. Rev. B **85**, 125127 (2012).
[24] D. J. Scalapino, S. R. White, and S. Zhang, Phys. Rev. B **47**, 7995 (1993).
[25] M. Vekic, S. R. White, Phys. Rev. B **47**, 1160-1163 (1993).